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## Testing Rationale

### Zinc Mercaptotoluimidazole

CAS Registry Number 61617-00-3

The R. T. Vanderbilt Company, Inc.  
P. O. Box 5150  
Norwalk, CT 06856-5150 USA

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### Summary

The R. T. Vanderbilt Company, Inc. is pleased to submit this test plan for zinc mercaptotoluimidazole (Vanox® ZMTI) for review and public comment under the Environmental Protection Agency's High Production Volume (HPV) Challenge Program.

Zinc mercaptotoluimidazole (ZMTI) is used as an antioxidant synergist in natural and synthetic rubber; it improves the performance of the primary antioxidant (such as a hindered phenol), allowing less to be used while maintaining effectiveness reducing the amount of primary antioxidant required to be effective. This use requires negligible water solubility, high organic/oil solubility and low vapor pressure. Existing data and use experience suggest little concern for mammalian toxicity, but structural similarity to other chemicals used in the rubber industry warrants additional testing. Therefore, we propose the following studies to meet the requirements of the EPA High Production Volume Chemical Testing Program:

- subchronic toxicity to rats with reproductive and developmental assessments
- aquatic toxicity (algal growth inhibition, acute toxicity to aquatic invertebrates and acute toxicity to aquatic vertebrates)
- ready biodegradability

**Aquatic Toxicology.** There are no data on the toxicity of ZMTI to aquatic organisms, and no biodegradability or bioaccumulation studies have been performed on ZMTI. Therefore, we propose an algal growth inhibition study and acute toxicity studies on aquatic invertebrates (*Daphnia magna*) and fish (rainbow trout, *Oncorhynchus mykiss*). We also propose a ready biodegradability study (OECD 301B).

**Acute Toxicity:** The acute oral LD<sub>50</sub> for ZMTI is 800 mg/kg. There are dermal and ocular irritation studies; ZMTI is not a skin irritant but is a slight eye irritant. The acute dermal LD<sub>50</sub> is greater than 2,000 mg/kg and the acute inhalation LC<sub>50</sub> is greater than 2.03 mg/l. ZMTI is a dermal sensitizer when tested by the Magnusson-Kligman method. We believe that the acute toxicity data for this material are acceptable and we propose no additional studies in this area.

**Mutagenicity:** We have conducted a bacterial reverse mutation assay (Ames test) as an initial screen. The results of this assay are negative (i.e., mutation frequency did not increase). The molecular structure does not suggest that it would be mutagenic in other assay systems; this is further supported by the fact that the molecule is used as an antioxidant synergist. Therefore, we do not believe that additional mutagenicity studies are warranted at this time.

**Repeated Dose Toxicity:** There are no subchronic toxicity, developmental toxicity or reproductive toxicity data on ZMTI. We propose a combined 28-day subchronic toxicity study with reproductive and developmental toxicity screens (OECD 422) to address this.

**Reproductive and Developmental Toxicity:** There are no developmental or reproductive toxicity data on ZMTI. We propose a combined 28-day subchronic toxicity study with reproductive and developmental toxicity screens (OECD 422) to address this.

**Conclusion:** The physical properties of zinc mercaptotoluimidazole have been adequately studied; however, additional data are required to meet the requirements of the EPA High Production Volume Challenge Program. Every effort has been made to select studies that will provide the most (and the most reliable) information using the fewest animals possible.

## Background Information: Manufacturing and Commercial Applications

### Manufacturing

Zinc mercaptotoluimidazole has been manufactured for over 30 years. It is manufactured by batch rather than continuous process. ZMTI is manufactured by converting 2-mercaptotoluimidazole to the insoluble zinc salt by reaction with zinc oxide.

### Commercial Applications

The largest commercial use of ZMTI is as an antioxidant synergist for natural and synthetic rubber. It is typically used at 0.5 to 1 part per every 100 parts of rubber (phr).

### Shipping/Distribution

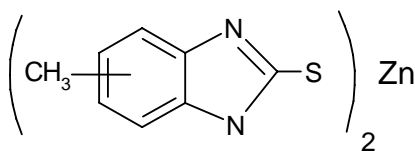
ZMTI is shipped extensively throughout the world from manufacturing plants located in North America and western Europe.

### Worker/Consumer Exposure

To the best of our knowledge, all ZMTI is used by the rubber industry, mostly by large industrial users as a component of their rubber compounds. The rubber and plastics additives industry has a long safety record and only sophisticated industrial users handle this material. It is available as a powder and as an aqueous dispersion; the powder is treated to minimize dust generation. Most large industrial users have mechanized materials handling systems, so employee exposure is minimal. The greatest potential for skin and inhalation exposure is at the packing station at the manufacturing site and, to a lesser extent, during weighing activities at the customer site. Nuisance dust is the primary source of worker exposure.

Consumer exposure is minimal. Small amounts are used in rubber processing, and the material becomes bound in the rubber matrix during vulcanization. The most likely route of consumer exposure is skin contact from rubber or latex articles. Skin irritation is unlikely but allergic skin reactions may occur.

### STRUCTURE



ZMTI is regulated for use in food-contact applications by the Food and Drug Administration:

FCN 000201: 2H-benzimidazole-2-thione, 1,3-dihydro-, 4(or 5)-methyl-, zinc salt (2:1) containing up to 4 percent by weight petroleum process oil: As an antioxidant synergist in natural or synthetic rubber gloves intended for repeat use in the meat packing industry. To be used in equal amounts with the primary currently regulated antioxidant, at no greater than 1 percent by weight of the rubber gloves.

# ZINC MERCAPTOTOLUIMIDAZOLE

## Test Plan

CAS No. 61617-00-3

R. T. Vanderbilt Company, Inc.  
December, 2002

Physical-Chemical					
Melting Point	Boiling Point	Vapor Pressure	Partition Coefficient	Water Solubility	
A	Calc	Calc	Calc	A	
Environmental Fate					
Photodegradation	Stability in Water	Transport/ Distribution	Biodegradation		
Calc	Calc	Calc	A		
Ecotoxicity					
Acute Toxicity to Fish		Acute Toxicity to Aquatic Plants (e.g., Algae)		Acute Toxicity to Aquatic Invertebrates (e.g., Daphnia)	
Test		Test		Test	
Mammalian Toxicity					
Acute Toxicity	Bacterial Genetic Toxicity <i>In Vitro</i>	Mammalian Genetic Toxicity <i>In Vivo</i>	Repeat Dose Toxicity	Reproductive Toxicity	Developmental Toxicity
A	A	NR (1)	Test	Test	Test

Legend	
Symbol	Description
Test	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NR	Not required per the OECD SIDS guidance
NA	Not applicable due to physical/chemical properties
SAR	Structure-Activity Relationship

(1) Mammalian genetic toxicity testing is generally not required if the results of *in vitro* mutagenicity tests are negative.